THE DICARBON BONDING PUZZLE

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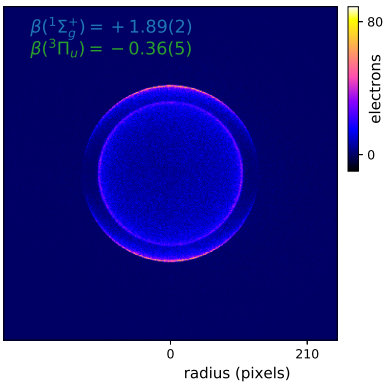
At first glance dicarbon, C_2, would appear to be a very simple homonuclear diatomic molecule. However the bonding structure of C_2 has long been a topic of debate, with different qualitative theories predicting a C−C bond order of 2, 3, or even 4[a]. Recent evidence for a quadruply bonded dicarbon has been provided by multiconfigurational *ab-initio* calculations[b]. However, the interpretation of these calculations has caused debate, with some research preferring the notion of a double, triple, or quasi double-triple bond, while other studies note that there is not enough evidence to clearly define the bonding nature of C_2[c].



In this work, photoelectron spectra of the C_2^- anion are measured using a high resolution photoelectron imaging (HR-PEI) spectrometer. The electron anisotropy of the detachment reveals the character of the parent anion orbital. Detachment to both the ground $\tilde{X}\,^1\Sigma_g^+$ and first excited $\tilde{a}^3\Pi_u$ electronic states is observed, identifying the character of two orbitals: the diffuse detachment orbital of the anion, and the HOMO of the neutral. The measurements show that electron detachment occurs from a pure s-like orbital ($3\sigma_g$) and a dominant p-like orbital ($1\pi_u$), that is inconsistent with the predictions of strongly mixed (50:50) sp orbitals required for the high bond order models, a result compatible only with the predictions of a C=C double bonding scheme.

[a] R. M. Macrae, *Sci. Prog.* **99**, 1 (2016)

[b] S. Shaik, D. Danovich, W. Wu, P. Su, H. Rzepa, P. Hiberty, *Nat. Chem.* **4**, 195 (2012)

[c] R. Zhong, M.Zhang, H. Xu, Z. Su, *Chem. Sci.* **7**, 1028 (2016)

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